10/821,500

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FULL ESTIMATED COST

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L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 12:45:03 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -12 TO ITERATE

100.0% PROCESSED

12 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L210 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL **ENTRY SESSION** 172.10 172.31

FULL ESTIMATED COST

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FILE COVERS 1907 - 4 Jun 2007 VOL 146 ISS 24
FILE LAST UPDATED: 3 Jun 2007 (20070603/ED)
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http://www.cas.org/infopolicy.html
=> s 12
L3
              4 L2
=> dup rem 13
PROCESSING COMPLETED FOR L3
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=> d 14 bib abs hitstr 1-4
L4
     ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ΑN
     2005:1103247 CAPLUS
DN
     143:382388
TI
     Fluorescent labeled nucleotide derivatives
     Shen, Gene G.-Y.; Lin, Yuan; Michael, Josephine M.
IN
PA
SO
     U.S. Pat. Appl. Publ., 19 pp.
     CODEN: USXXCO
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                      DATE
                          ____
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                                              -----
     US 2005227240
                           A1
                                  20051013
                                              US 2004-821500
                                                                       20040409
     WO 2005103162
                           A1
                                  20051103
                                              WO 2005-US9330
                                                                       20050322
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
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              RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
     EP 1732989
                                  20061220
                                             EP 2005-725978
                           A1
                                                                       20050322
         R: DE, FR, GB
PRAI US 2004-821500
                                  20040409
                           Α
     WO 2005-US9330
                           W
                                  20050322
os
     MARPAT 143:382388
AB
     Fluorescent labeled reporter compds. having a modified cyanine dye that is
     coupled to a nucleotide derivative through a linker are disclosed.
     compds. are useful for nucleic acid sequence anal. The fluorescent
     labeled reporter compds. are ring-locked cyanine dyes that are coupled to
     a nucleotide derivative, such as a modified DNA base, through a linker.
     fluorescent labeled reporter compds. can be used as DNA chain-terminators
     in DNA synthesis to generate DNA fragments that are fluorescently-labeled
     at the 3'-terminal end of the DNA fragment.
ΙT
     866560-82-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (ddATP-RLDBCy7; fluorescent labeled nucleotide derivs. for DNA
        sequencing)
RN
     866560-82-9 CAPLUS
     3H-Indolium, 2-[2-[2-[4-[2-[[[3-[6-amino-9-[(2R,5S)-5-(3,5,7,7-1])]]]]])
CN
     tetrahydroxy-3,5,7-trioxido-2,4,6-trioxa-3,5,7-triphosphahept-1-yl)-2-
```

furanyl]-7H-purin-5-yl]-2-propynyl]amino]carbonyl]amino]ethyl]phenoxy]-3[2-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2ylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-1-ethyl-3,3-dimethyl-5sulfo-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-B

ΙT 866560-81-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (ddCTP-RLCy7; fluorescent labeled nucleotide derivs. for DNA sequencing) RN866560-81-8 CAPLUS CN 3H-Indolium, 2-[2-[2-[4-[2-[[[[3-[4-amino-1,2-dihydro-2-oxo-1-[(2R,5S)tetrahydro-5-(3,5,7,7-tetrahydroxy-3,5,7-trioxido-2,4,6-trioxa-3,5,7triphosphahept-1-yl)-2-furanyl]-5-pyrimidinyl]-2propynyl]amino]thioxomethyl]amino]ethyl]phenoxy]-3-[2-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)ethylidene]-1-cyclohexen-1yl]ethenyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-B

RN 866560-78-3 CAPLUS

CN 3H-Indolium, 1-ethyl-2-[2-[3-[(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)ethylidene]-2-[4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-, inner salt (9CI) (CA INDEX NAME)

$$S = C = N - CH_2 - CH_2$$

$$Me$$

$$Me$$

$$CH - CH$$

$$CH - CH$$

$$Et$$

$$SO_3$$

IT 866560-80-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(ring-locked DBCy7; fluorescent labeled nucleotide derivs. for DNA sequencing)

RN 866560-80-7 CAPLUS

CN 1H-Benz[e]indolium, 3-ethyl-2-[2-[3-[(3-ethyl-1,3-dihydro-1,1-dimethyl-7-sulfo-2H-benz[e]indol-2-ylidene)ethylidene]-2-[4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-1,1-dimethyl-7-sulfo-, inner salt (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:441785 CAPLUS

DN 137:211531

TI Optimization of sequencing conditions using near-infrared lifetime identification methods in capillary gel electrophoresis

AU Lassiter, Suzanne J.; Stryjewski, Wieslaw; Owens, Clyde V.; Flanagan, James H., Jr.; Hammer, Robert P.; Khan, Shaheer; Soper, Steven A.

CS Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA

SO Electrophoresis (2002), 23(10), 1480-1489 CODEN: ELCTDN; ISSN: 0173-0835

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

AB We have investigated the sample preparation and electrophoresis conditions necessary to prepare DNA sequencing samples appropriate for use with near-IR (IR) fluorescent labels with dye identification accomplished via lifetime techniques. It was found that several sample preparation protocols required attention to maximize the fluorescence yields of the labeling dyes, such as thermal cycling conditions, choice of counter ion used for the ethanol precipitation step and also, dye-primer vs. dye terminator chemistries. In addition,

several different sieving matrixes were investigated for their effects on both the fluorescence properties of the labeling dyes and electrophoretic resolution Extended times used for the high temperature denaturing of duplexed DNA

fragments during cycle sequencing produced cleavage products, in which the covalently attached dye to the sequencing primer was released through attack by dithiothreitol (DTT). Even under optimized thermal cycling conditions, free dye was generated that masked readable data from the sequencing traces. Ethanol precipitation was necessary to remove this free dye with the proper choice of counter ion (sodium). The results using different sieving matrixes indicated that linear polyacrylamides (LPAs) were appropriate for any fluorescence measurement, since they could readily be replaced between runs minimizing deleterious memory effects

associated with cross-linked polyacrylamide gels. After investigation of several different sieving LPAs, the com. available POP6 was found to be particularly attractive, since it produced good electrophoretic resolution, single exponential behavior for the near-IR dye series investigated herein, and also, discernible lifetime differences within the dye set. Finally, dye-terminator chemical was also found to minimize bleeding in the gel matrix produced by large amts. of unextended dye-primer within the gel lane.

TΤ 209911-58-0 209911-61-5 209911-65-9 209911-69-3

> RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(optimization of sequencing conditions using near-IR lifetime identification methods in capillary gel electrophoresis)

RN

209911-58-0 CAPLUS
3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-CN 2-ylidene]ethylidene]-2-[2-iodo-4-(2-isothiocyanatoethyl)phenoxy]-1cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-61-5 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-bromo-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3-isothiocyanatoethyl)phenoxy]-3-[[1,3-isothiocyanatoethyl]phenoxy]-3-[[1,3-isothiocydihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-65-9 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-chloro-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt,

RN 209911-69-3 CAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[2-fluoro-4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

## RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1998:341978 CAPLUS

DN 129:104816

TI Near-infrared heavy-atom-modified fluorescent dyes for base-calling in DNA-sequencing applications using temporal discrimination

AU Flanagan, James H., Jr.; Owens, Clyde V.; Romero, Sarah E.; Waddell, Emanuel; Kahn, Shaheer H.; Hammer, Robert P.; Soper, Steven A.

CS Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA

SO Analytical Chemistry (1998), 70(13), 2676-2684 CODEN: ANCHAM; ISSN: 0003-2700

PB American Chemical Society

DT Journal

LA English

AB A series of near-IR fluorescent dyes were prepared which contained an intramol. heavy atom for altering the fluorescence lifetimes to produce a set of probes appropriate for base-calling in a single-lane DNA sequencing format. The heavy-atom modification consisted of an intramol. halogen situated on a remote section of the chromophore in order to minimize the

perturbation on the lifetimes and fluorescence quantum yields. In addition, the dye series possessed an isothiocyanate functional group to allow facile attachment to sequencing primers. The unconjugated dyes showed similar absorption and emission maxima ( $\lambda abs = 765-768 \text{ nm}$ ;  $\lambda$ em = 794-798 nm) as well as fluorescence quantum yields that were invariant, within exptl. error, with the heavy atom. However, the lifetimes of these dyes were found to vary with the identity of the halogen substitution (I,  $\tau f = 947$  ps; F,  $\tau f = 843$  ps, measured in methanol), with an average variation within the dye series of 35 ps. spectroscopic properties of the free dyes and the dyes conjugated to sequencing primers on the 5'-end of the oligonucleotide were determined in a DNA-sequencing matrix (denaturing gels containing formamide). The results indicated slight differences in the fluorescence properties of the free dyes compared to those of the dye/primer conjugates in this particular Inspection of the ground-state absorption spectra showed significant aggregation for the free dyes in this solution, but the conjugated dyes exhibited no sign of aggregation due to the highly anionic nature of the oligonucleotide. The fluorescence lifetimes of the dye/primer conjugates demonstrated lifetimes which ranged from 735 to 889 ps, with an average variation of 51 ps, an adequate difference to allow facile discrimination of these dyes in DNA-sequencing conditions. In addition, the free solution electrophoretic mobilities of the native heavy-atom-modified dyes were found to be very similar. When the dye/primer conjugates were electrophoresed in a cross-linked polyacrylamide gel electrophoresis capillary column, they comigrated, indicating that, in single-lane sequencing applications, when utilizing these dyes, no postrun corrections would be required to correct for dye-dependent mobility shifts. 209911-58-0DP, oligodeoxyribonucleotide conjugates 209911-58-0P 209911-61-5DP, oligodeoxyribonucleotide conjugates 209911-61-5P 209911-65-9DP, oligodeoxyribonucleotide conjugates 209911-65-9P 209911-69-3DP, oligodeoxyribonucleotide conjugates 209911-69-3P RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses) (near-IR heavy-atom-modified fluorescent dyes for base-calling in DNA-sequencing applications using temporal discrimination)

209911-58-0 CAPLUS
3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[2-iodo-4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-58-0 CAPLUS

ΙT

ŔN

CN

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[2-iodo-4-(2-isothiocyanatoethyl)phenoxy]-1-

cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt,
ion(1-) (9CI) (CA INDEX NAME)

RN 209911-61-5 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-bromo-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-61-5 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-bromo-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-65-9 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-chloro-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-65-9 CAPLUS

CN 3H-Indolium, 2-[2-[2-[2-chloro-4-(2-isothiocyanatoethyl)phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN 209911-69-3 CAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[2-fluoro-4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RN

209911-69-3 CAPLUS 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-CN 2-ylidene]ethylidene]-2-[2-fluoro-4-(2-isothiocyanatoethyl)phenoxy]-1cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

ΙT 209911-55-7P

RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (near-IR heavy-atom-modified fluorescent dyes for base-calling in DNA-sequencing applications using temporal discrimination)

209911-55-7 CAPLUS RN

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-) (9CI) (CA INDEX NAME)

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:575537 CAPLUS

DN 127:231448

TI Functionalized Tricarbocyanine Dyes as Near-Infrared Fluorescent Probes for Biomolecules

AU Flanagan, James H., Jr.; Khan, Shaheer H.; Menchen, Steve; Soper, Steven A.; Hammer, Robert P.

CS Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA

SO Bioconjugate Chemistry (1997), 8(5), 751-756 CODEN: BCCHES; ISSN: 1043-1802

PB American Chemical Society

DT Journal

LA English

OS CASREACT 127:231448

The syntheses of 3 novel functionalized tricarbocyanine dyes are described. These dyes containing isothiocyanate and succinimidyl ester functional groups are reactive toward primary amines and can be used as fluorescent probes for biol. pertinent compds. such as amino acids and functionalized dideoxynucleotides. The absorption and fluorescence maxima occur in the near-IR regin of the spectrum (770-820 nm). The succinimidyl ester proved to be very sensitive to hydrolysis and was generated in situ to label amino acids and alkyl amines. The isothiocyanates were less susceptible to hydrolysis and were conjugated using organic modified [40% (volume/volume) acetonitrile] buffers to amino acids. A dye with an alkyl isothiocyanate moiety showed conjugation to amino-functionalized dideoxynucleotide triphosphates.

IT 195382-08-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(functionalized tricarbocyanine dyes as near-IR fluorescent probes for biomols.)

RN 195382-08-2 CAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-2-[4-(2-isothiocyanatoethyl)phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-(3-sulfopropyl)-, inner salt, ion(1-), (all-E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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